

Structural Distortion Stabilizing the Antiferromagnetic and Semiconducting Ground State of BaMn_2As_2

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We report evidence that the experimentally found antiferromagnetic structure as well as the semiconducting ground state of BaMn_2As_2 are caused by optimally-localized Wannier states of special symmetry existing at the Fermi level of BaMn_2As_2 . In addition, we find that a (small) tetragonal distortion of the crystal is required to stabilize the antiferromagnetic semiconducting state. To our knowledge, this distortion has not yet been established experimentally.

Keywords: BaMn_2As_2 , magnetism, small band gap semiconductor, nonadiabatic Heisenberg model, group theory

I. INTRODUCTION

The electronic ground state of BaMn_2As_2 shows resemblances but also striking differences, as compared with the ground state of the isostructural compound BaFe_2As_2 . Both materials become antiferromagnetic below the respective Néel temperature. However, while the magnetic moments in BaMn_2As_2 are orientated along the tetragonal c axis [1], see Fig. 1, they are orientated perpendicular to this axis in BaFe_2As_2 [2].

Also very interesting is the observation that, unlike BaFe_2As_2 , BaMn_2As_2 is a small band gap antiferromagnetic *semiconductor* [3, 4]. No structural transformation or distortion of BaMn_2As_2 in this antiferromagnetic semiconducting state was experimentally detected [1].

The present paper reports evidence that the remarkable features of the electronic ground state of BaMn_2As_2 are connected with optimally-localized Wannier functions existing at the Fermi level of BaMn_2As_2 . These Wannier functions are adapted to the symmetry of the antiferromagnetic structure and constructed from Bloch functions of well-defined symmetry forming narrow “magnetic bands” as defined in Ref. [5] (see Definition 16 *ibidem*).

In Section II.1 we shall identify the tetragonal space group $I\bar{4}2m$ (121) as the space group of the antiferromagnetic structure observed in BaMn_2As_2 (the number in parenthesis is the international number) and determine the magnetic group M_{121} of this structure. We will show that no magnetic band related to M_{121} exists in the band structure of BaMn_2As_2 . The situation changes drastically when in Section II.2 we shall consider a slightly distorted crystal. We will define and verify the existence of a magnetic “super” band in distorted antiferromagnetic BaMn_2As_2 . This super band consists of three magnetic bands as defined in Ref. [5] with Wannier functions situated at the Ba, the Mn, and the As atoms, respectively.

Our group-theoretical results in Section II will be physically interpreted in Section III. We will argue in Section III.1 that a small tetragonal distortion of the crystal is required to stabilize the antiferromagnetic semiconducting ground state of BaMn_2As_2 . This distortion

alters the space group $I\bar{4}2m = \Gamma_q^v D_{2d}^{11}$ of the undistorted antiferromagnetic crystal into the space group $P\bar{4}2_1c = \Gamma_q^4 D_{2d}^4$ (which is still tetragonal) and may be realized by the displacements of the Mn atoms depicted in Fig. 1 (b). These displacements are evidently so small that they have not yet been experimentally verified [1]. In Section III.2 we shall show that evidently the magnetic super band is responsible for the small band gap in the antiferromagnetic semiconducting ground state, and in Section III.3 why the space groups of the magnetic structures in BaFe_2As_2 and BaMn_2As_2 differ so strikingly.

I.1. Nonadiabatic Heisenberg model

The existence of magnetic bands in the band structure of BaMn_2As_2 is physically interpreted within the nonadiabatic Heisenberg model (NHM) [6]. The second postulate of the NHM (Equation (2.19) of [6]) states that in narrow bands (i.e. in band satisfying Equation (2.13) of [6]) the electrons may lower their total correlation energy by condensing into an atomic-like state as it was described by Mott [7] and Hubbard [8]: the electrons occupy the localized states as long as possible and perform their band motion by hopping from one atom to another. Within the NHM, however, the localized states *are not represented by (hybrid) atomic orbitals but consequently by symmetry-adapted optimally-localized Wannier states*. The electrons are strongly correlated in this atomic-like state, leading to the consequence that a consistent description of the localized Wannier states must involve the nonadiabatic motion of the atomic cores [6].

Hence, the nonadiabatic localized functions representing these nonadiabatic Wannier states depend on an additional coordinate characterizing the motion of the atomic cores. Fortunately, these mathematically complicated functions need not be explicitly known. They can be simply managed within the group-theoretical NHM because they have the same symmetry as the related adiabatic optimally-localized Wannier functions as defined in Ref. [5]. In this context we speak of “adiabatic” Wan-

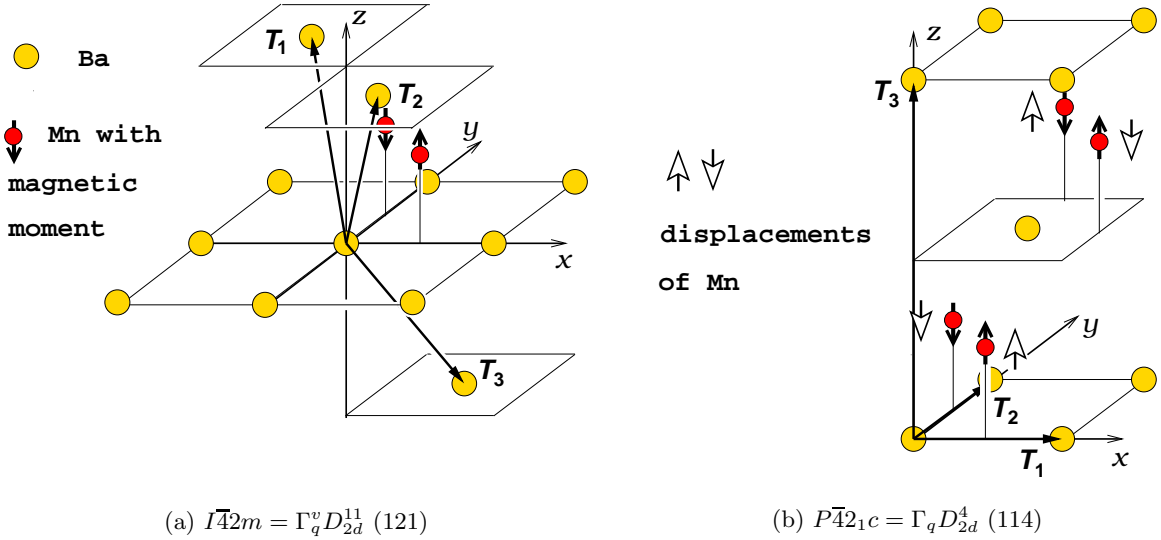


FIG. 1. Experimentally observed [1] antiferromagnetic structure in undistorted (a) and distorted (b) BaMn_2As_2 . While sufficient Ba atoms are depicted to recognize the orientation of the crystal, the Mn atoms are shown only within the respective unit cell. The As atoms are not included. The indicated (small) displacements of the Mn atoms in exact $\pm\mathbf{T}_3$ direction realize the tetragonal primitive space group $P\bar{4}2_1c$.

nier functions if they do not dependent on the nonadiabatic motion of the atomic cores.

The total correlation energy of the electron system decreases by the nonadiabatic condensation energy ΔE defined in Equation (2.20) of [6] at the condensation into the nonadiabatic atomic-like state.

II. MAGNETIC BANDS IN THE BAND STRUCTURE OF BaMn_2As_2

II.1. The space group $I\bar{4}2m$ (121) of the antiferromagnetic structure in undistorted BaMn_2As_2

Removing from the space group $I4/mmm$ of BaMn_2As_2 all the symmetry operations not leaving invariant the magnetic moments of the Mn atoms, we obtain the group $I\bar{4}2m$ (121) as the space group of the antiferromagnetic structure in undistorted BaMn_2As_2 . Just as $I4/mmm$, the group $I\bar{4}2m$ has the tetragonal body-centered Bravais lattice Γ_q^v .

The group $I\bar{4}2m$ may be defined by the two “generating elements”

$$\{S_{4z}^+|000\} \text{ and } \{C_{2x}|000\}, \quad (1)$$

see Table 3.7 of Ref. [9]. Just as in all our papers, we write the symmetry operations $\{R|pqr\}$ in the Seitz notation detailed in the textbook of Bradley and Cracknell [9]: R stands for a point group operation (as defined, e.g., in Table 1.4 *ibidem*) and pqr denotes the subsequent translation $\mathbf{t} = p\mathbf{T}_1 + q\mathbf{T}_2 + r\mathbf{T}_3$, where the $\mathbf{T}_1, \mathbf{T}_2$, and \mathbf{T}_3 denote

the basic vectors of the respective Bravais lattice given in Fig. 1. A (magnetic) structure is invariant under a space group G if it is already invariant under the generating elements of G . The two generating symmetry operations (1) leave invariant the atoms of BaMn_2As_2 since both operations are elements of $I4/mmm$. By means of Fig. 1 (a) we can realize that they additionally leave invariant the magnetic structure, cf. Sec. 3.1 of Ref. [10].

The associated magnetic group reads as

$$M_{121} = I\bar{4}2m + \{KI|000\}I\bar{4}2m, \quad (2)$$

where K and I denote the operator of time inversion and the inversion, respectively. $\{KI|000\}$ leaves invariant both the atoms and the magnetic structure since $\{I|000\} \in I4/mmm$.

With consideration of the change of symmetry by the magnetostriction, but neglecting all other magnetic interactions, we receive from the band structure of BaMn_2As_2 given in Fig. 2 the band structure of antiferromagnetic undistorted BaMn_2As_2 depicted in Fig. 3. All the possible magnetic bands (Definition 16 of Ref. [5]) in the magnetic group M_{121} are listed in Table 3. The “best” magnetic band would be band 2 of Mn as highlighted in Fig. 3 by the red labels.

Band 2 of Mn, however, is not a magnetic band in BaMn_2As_2 because it misrepresents the Bloch functions at parts of the Fermi level. Between the N_1 and P_3 states it jumps over the Fermi level simulating in this way Bloch states at the Fermi level which do not exist. The same situation we have between the Z_5 state and the two X_3, X_1 states. Along the lines Γ, Σ the Γ_5 state is connected with

Energy (eV)

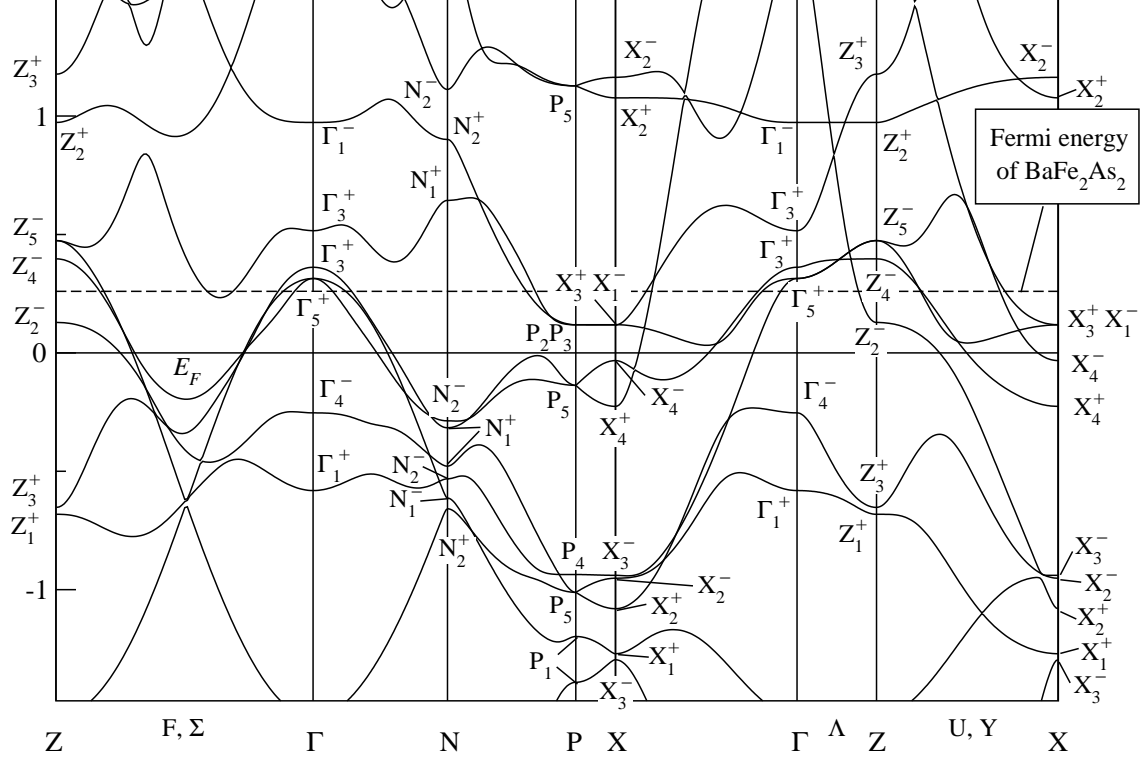


FIG. 2. Band structure of BaMn_2As_2 as calculated by the FHI-aims program [11, 12], using the structure parameters given in Ref. [1]. The space group of BaMn_2As_2 is the tetragonal group $I4/mmm$ (139) [1], the given symmetry labels are determined by the author. The notations of the points and lines of symmetry in the Brillouin zone for Γ_q^v follow Fig. 3.10 (b) of Ref. [9], and the symmetry labels are defined in Table 2 of Ref. [13]. E_F denotes the Fermi level. The band structure of BaMn_2As_2 essentially coincides with the band structure of BaFe_2As_2 (depicted in Fig. 2 of Ref. [13]) when the Fermi level is moved upwards to the dashed line.

two Bloch states at the Fermi level, which, however, are not connected to Z_5 .

We could try to render ineffective these unfavorable jumps by adding further bands to the Mn band as it will be successful in the space group $P\bar{4}2_1c$ considered in the following Section II.2. By means of Table 3 we may satisfy ourselves that this procedure is not possible. For instance, we neither can add band 1 nor band 2 of As to band 2 of Mn because there is neither a Γ_4 state nor an additional P_3 state available in the band structure.

II.2. The space group $P\bar{4}2_1c$ (114) of the antiferromagnetic structure in distorted BaMn_2As_2

The situation described in the preceding Section II.1 changes drastically when we consider the space group $P\bar{4}2_1c$. This group has no longer the tetragonal body-centered Bravais lattice Γ_q^v , but the tetragonal primitive lattice Γ_q and may be defined by the two generating elements

$$\{S_{4z}^+|000\} \text{ and } \{C_{2x}|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \quad (3)$$

see Table 3.7 of Ref. [9] (note that the basis vectors now are given in Fig. 1 (b)). As well as the generating elements of $I\bar{4}2m$ (1) they leave invariant both the positions of the atoms and the magnetic structure since the vector $\mathbf{t} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ is a lattice vector in Γ_q^v . In addition, the generating elements (3) leave invariant the displacements of the Mn atoms depicted in Fig. 1 (b). Thus these displacements “realize” the space group $P\bar{4}2_1c$ in the sense that the electrons now move in a potential adapted to the symmetry of the distorted crystal. The group $P\bar{4}2_1c$ represents only a small distortion of the crystal because it is still tetragonal and possesses the same point group as the space group $I\bar{4}2m$ of antiferromagnetic undistorted BaMn_2As_2 . It is only the translation $\mathbf{t} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ which is no longer a symmetry operation in $P\bar{4}2_1c$.

At first, the two anti-unitary operations $\{KI|000\}$ and $\{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ may define the magnetic group of the magnetic structure since both operations leave invariant the magnetic structure. However, only $\{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ leaves additionally invariant the displacement of the Mn atoms depicted in Fig 1 (b). These displacements, however, are required to realize the space group $P\bar{4}2_1c$. Hence, the magnetic group of antiferromagnetic distorted BaMn_2As_2

Energy (eV)

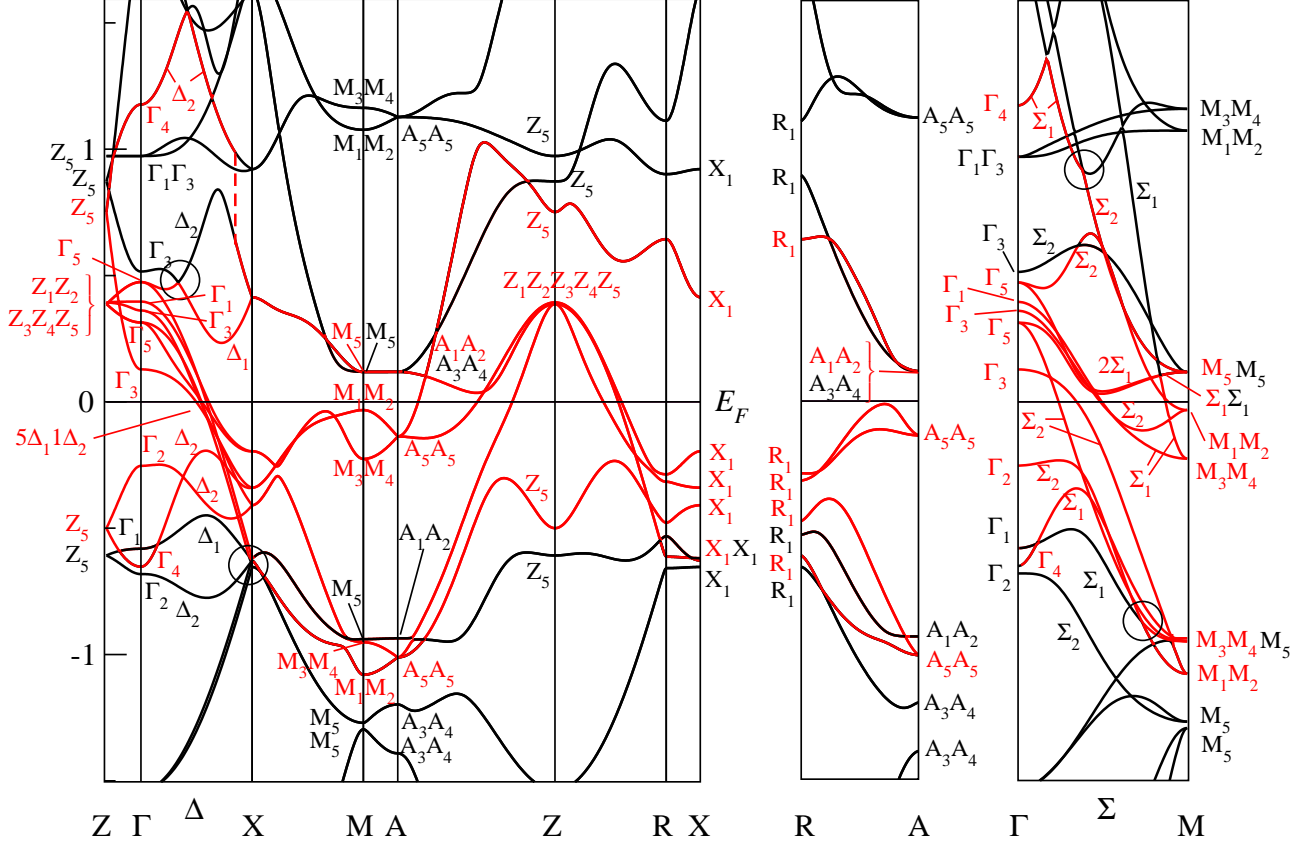


FIG. 4. The band structure of BaMn_2As_2 as given in Fig. 2 folded into the Brillouin zone for the tetragonal primitive Bravais lattice Γ_q of the space group $P\bar{4}2_1c$ (114). The symmetry labels are defined in Table 4 and are determined from Fig. 2 by means of Table 5. The notations of the points of symmetry follow Fig. 3.9 of Ref. [9]. E_F denotes the Fermi level. The red lines and red symmetry labels form the magnetic “super” band of the experimentally observed [1] antiferromagnetic structure in BaMn_2As_2 . It is related to *all* the atoms of BaMn_2As_2 , that means that it is related to two Ba, four Mn and four As atoms in the unit cell of Γ_q , and, hence, consists of ten branches. Whenever a black and a red line overlap, the red line lies on the top. The four circles mark the regions with transitions from Δ_2 to Δ_1 , Δ_1 to Δ_2 , Σ_1 to Σ_2 , and Σ_2 to Σ_1 , respectively, on the lines Δ and Σ . These transitions slightly destroy the symmetry of related the Wannier functions in the space group $P\bar{4}2_1c$. However, since these transitions only occur in two lines of two branches far away from the Fermi level, we assume that we may describe the magnetic structure of BaMn_2As_2 with high accuracy in the space group $P\bar{4}2_1c$. Nevertheless, these transitions produce a small additional distortion of the crystal going beyond the distortion depicted in Fig. 1 (b).

II.3. Time-inversion symmetry

The time-inversion symmetry is no essential object in antiferromagnetic BaMn_2As_2 : all the three space groups $I4/mmm$ (139), $P\bar{4}2_1c$ (114), and $P\bar{4}$ (81) possess one-dimensional representations allowing a *stable* magnetic state with the magnetic group M_{121} (2), M_{114} (4), and M_{81} (6), respectively, see Tables 1, 4, and 7 and the notes to these tables. Consequently, time-inversion symmetry influences neither the antiferromagnetic structure nor the structural distortions in BaMn_2As_2 (as it is the case, for instance, in BaFe_2As_2 [13]). Time-inversion symmetry only forbids magnetic moments located at the As atoms, see Note (x) of Table 6.

III. PHYSICAL INTERPRETATION

The existence and the properties of the roughly half-filled magnetic super band in the band structure of BaMn_2As_2 yield to an understanding of three phenomena that shall be considered in this section:

- the experimentally observed [1] antiferromagnetic order together with a structural distortion not yet experimentally found;
- the semiconducting ground state; and
- the different magnetic structures in BaMn_2As_2 and BaFe_2As_2 .

III.1. The antiferromagnetic order and the structural distortion in BaMn_2As_2

In a material possessing a narrow, roughly half-filled magnetic band or super band related to a magnetic group M , the NHM defines a nonadiabatic Hamiltonian H^n representing atomic-like electrons (Section I.1) within this band [6]. An important feature of H^n is that it only commutes with the symmetry operations of M , but *does not commute* with the remaining symmetry operations of the paramagnetic group of the crystal (this follows from the fact that the optimally-localized Wannier functions in a magnetic band may be chosen symmetry-adapted to M , but cannot be chosen symmetry-adapted to the complete paramagnetic group, cf. Section 1 of Ref. [5]).

Thus, the electrons in such a narrow, roughly half-filled magnetic band or super band may gain the nonadiabatic condensation energy ΔE (Section I.1) by condensing into an atomic-like state only if the electrons really move in a potential with the magnetic group M , that is, only if a magnetic structure with the magnetic group M really exists. As a consequence, the electrons *activate* in the nonadiabatic system a spin dependent exchange mechanism producing a magnetic structure with the magnetic group M [14, 15].

In the case of BaMn_2As_2 , the group $I\bar{4}2m$ (121) is the space group of the antiferromagnetic structure in *undistorted* BaMn_2As_2 . However, within this group there does not exist a magnetic band, see Sec. II.1. Indeed, a magnetic band, even a magnetic super band, exists in the space group $P\bar{4}2_1c$ (114) of distorted BaMn_2As_2 , see Sec. II.2.

Hence, in BaMn_2As_2 the electron system cannot condense into the atomic-like state by the production of the magnetic structure *alone* but must additionally produce a spatial distortion of the crystal realizing - together with the magnetic structure - the magnetic group M_{114} (4). This is achieved by the displacements of the Mn atoms depicted in Fig. 1 (b). Consequently, the magnetically ordered ground state of BaMn_2As_2 is accompanied by the displacements of the Mn atoms depicted in Fig. 1 (b).

III.2. The semiconducting ground state of BaMn_2As_2

The magnetic super band defines not only Wannier functions situated at *all the* atoms of BaMn_2As_2 , but it also comprises *all the Bloch states* at the Fermi level, see Fig. 4. Thus, if the magnetic super band is *exactly* half filled, the nonadiabatic Hamiltonian H^n produces very specific atomic-like electrons: at *any* atom of BaMn_2As_2 there exists a localized Wannier state occupied by exactly one electron and besides these atomic-like electrons there do not exist band-like electrons which would be able to transport electrical current. Thus, H^n possesses a semiconducting ground state since the atomic-like state

is separated from any band-like state by the nonadiabatic condensation energy ΔE mentioned in Section I.1. The experimental observation of an insulating ground state in BaMn_2As_2 suggests that, indeed, the magnetic super band is exactly half-filled.

III.3. Different magnetic structures in BaMn_2As_2 and BaFe_2As_2

While both compounds BaMn_2As_2 and BaFe_2As_2 exhibit an antiferromagnetic ordering below the respective Néel temperature, the space groups of the magnetic structures are quite different: in BaMn_2As_2 the space group of the magnetic structure is the tetragonal group $P\bar{4}2_1c$ (114) with magnetic moments oriented along the tetragonal c axis, and in BaFe_2As_2 it is the orthorhombic group $Cmca$ with magnetic moments orientated perpendicular to the c axis, see Fig. 1 of [1] and Fig. 3 of [2], respectively.

This surprising experimental observation can be understood comparing the band structures of both compounds as given in Fig. 2 and Fig. 2 of Ref. [13]. The band structure of BaFe_2As_2 is very similar to the band structure of BaMn_2As_2 , the essential difference is the position of the Fermi level: we may approximate the band structure of BaFe_2As_2 by the band structure of BaMn_2As_2 by shifting the Fermi level upwards by about 0.3 eV as it is indicated in Fig. 2.

A magnetic (super) band may be physically active only if the band is nearly half-filled. The band width of the (red) magnetic super band in Fig. 4 may be approximated by 2σ , where

$$\sigma = \sqrt{\frac{1}{N} \sum_{\mathbf{k}} (E_{\mathbf{k}} - E_F)^2} \approx 0.5 \text{ eV}, \quad (7)$$

denotes the standard deviation of the $N = 6 \cdot 10$ energy values $E_{\mathbf{k}}$ in the six points of symmetry of the magnetic super band.

Thus, the Fermi level is shifted in BaFe_2As_2 nearly to the top of the magnetic super band. Hence, in BaFe_2As_2 this band is far from being half-filled and determines neither the magnetic structure nor produces an isolating ground state in BaFe_2As_2 . Instead, the magnetic structure in BaFe_2As_2 is determined by the nearly half-filled magnetic band presented in Fig. 3 of Ref. [13] which is related to the space group $Cmca$ of the magnetic structure experimentally found in BaFe_2As_2 [2].

IV. CONCLUSIONS

This paper emphasizes the importance of the nonadiabatic condensation energy ΔE defined in Equation (2.20) of Ref. [6] (and already mentioned in Section I.1) which is evidently responsible for the striking electronic features of BaMn_2As_2 . ΔE is released at the transition from an

adiabatic band-like motion of the electrons to the nonadiabatic strongly-correlated atomic-like motion.

This finding is in accordance with former observations on a great number of superconducting and magnetic materials (see Section 1 of [5]) suggesting that superconductivity and magnetism are always connected with superconducting (Definition 22 of Ref. [5]) and magnetic bands, respectively. Thus, in superconducting and magnetic bands, the nonadiabatic condensation energy ΔE may evidently produce superconductivity and mag-

netism, respectively, and in some cases even a small band gap semiconductor.

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Appendix: Group-theoretical tables

This appendix provides Tables 1 – 7 along with notes to the tables.

TABLE 1. Character tables of the irreducible representations of the tetragonal space group $I\bar{4}2m = \Gamma_q^v D_{2d}^{11}$ (121) of the experimentally observed [1] antiferromagnetic structure in BaMn_2As_2 .

$\Gamma(000), Z(\frac{1}{2}\frac{1}{2}\frac{1}{2})$								$P(\frac{1}{4}\frac{1}{4}\frac{1}{4})$								$X(00\frac{1}{2})$					$N(0\frac{1}{2}0)$										
				S_{4z}^-	C_{2y}	σ_{da}						S_{4z}^-	C_{2y}	σ_{da}						E	C_{2z}	σ_{db}	σ_{da}				E	C_{2y}			
K	KI	E	C_{2z}	S_{4z}^+	C_{2x}	σ_{db}		K	KI	E	C_{2z}	S_{4z}^+	C_{2x}	σ_{db}		X_1	1	1	1	1		N_1	1	1				N_2	1	-1	
Γ_1, Z_1	(a)	(a)	1	1	1	1	1	P_1	(x)	(a)	1	1	1	1	1		X_3	1	1	-1	-1		N_2	1	-1						
Γ_2, Z_2	(a)	(a)	1	1	1	-1	-1	P_2	(x)	(a)	1	1	1	-1	-1		X_2	1	-1	1	-1										
Γ_3, Z_3	(a)	(a)	1	1	-1	1	-1	P_3	(x)	(a)	1	1	-1	1	-1		X_4	1	-1	-1	1										
Γ_4, Z_4	(a)	(a)	1	1	-1	-1	1	P_4	(x)	(a)	1	1	-1	-1	1																
Γ_5, Z_5	(a)	(a)	2	-2	0	0	0	P_5	(x)	(a)	2	-2	0	0	0																

Notes to Table 1

- (i) The notations of the points of symmetry follow Fig. 3.10 (b) of Ref. [9].
- (ii) The character tables are determined from Table 5.7 of Ref. [9].
- (iii) K denotes the operator of time inversion. The entry (a) indicates that the related corepresentations of the magnetic groups $I\bar{4}2m + \{K|000\}I\bar{4}2m$ and $I\bar{4}2m + \{KI|000\}I\bar{4}2m$ follow case (a) as defined in equation (7.3.45) of Ref. [9] (and determined by equation (7.3.51) of Ref. [9]). This information is interesting only in symmetry points invariant under the complete space group. (x) indicates that K does not leave invariant the point P .
- (iv) The one-dimensional representations at point P would be possible representations of a *stable* antiferromagnetic state because they comply with the demands in Section III C of Ref. [14].

TABLE 2. Compatibility relations between the Brillouin zone for the space group $I4/mmm$ (139) of paramagnetic BaMn_2As_2 and the Brillouin zone for the space group $I\bar{4}2m$ (121) of the antiferromagnetic structure in undistorted BaMn_2As_2 .

$\Gamma(000)$										$N(0\frac{1}{2}0)$				$X(00\frac{1}{2})$							
Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	N_1^+	N_1^-	N_2^+	N_2^-	X_1^+	X_2^+	X_3^+	X_4^+	X_1^-	X_2^-	X_3^-	X_4^-
Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_3	Γ_4	Γ_1	Γ_2	Γ_5	N_1	N_1	N_2	N_2	X_1	X_4	X_3	X_2	X_3	X_2	X_1	X_4

$Z(\frac{1}{2}\frac{1}{2}\bar{1})$										$P(\frac{1}{4}\frac{1}{4}\frac{1}{4})$				
Z_1^+	Z_2^+	Z_3^+	Z_4^+	Z_5^+	Z_1^-	Z_2^-	Z_3^-	Z_4^-	Z_5^-	P_1	P_2	P_3	P_4	P_5
Z_1	Z_2	Z_3	Z_4	Z_5	Z_3	Z_4	Z_1	Z_2	Z_5	P_1	P_2	P_3	P_4	P_5

Notes to Table 2

- (i) The Brillouin zone for $I\bar{4}2m$ is identical to the Brillouin zone for $I4/mmm$.
- (ii) The upper rows list the representations of the little groups of the points of symmetry in the Brillouin zone for $I4/mmm$. The lower rows list representations of these groups in $I\bar{4}2m$.
The representations in the same column are compatible in the following sense: Bloch functions that are basis functions of a representation \mathbf{D}_i in the upper row can be unitarily transformed into the basis functions of the representation given below \mathbf{D}_i .
- (iii) The notations of the representations are defined in Table 2 of Ref. [13] and Table 1, respectively.

TABLE 3. Representations at the points of symmetry in the space group $I\bar{4}2m = \Gamma_q^v D_{2d}^{11} (121)$ of all the energy bands of antiferromagnetic BaMn_2As_2 with symmetry-adapted and optimally localized Wannier functions centered at the Mn, As, and Ba atoms, respectively.

Mn	$\text{Mn}(\frac{1}{4}\frac{3}{4}\frac{1}{2})$	$\text{Mn}(\frac{3}{4}\frac{1}{4}\frac{1}{2})$	KI	Γ	P	Z	X	N
Band 1	\mathbf{d}_1	\mathbf{d}_1	OK	$\Gamma_1 + \Gamma_2$	P_5	$Z_3 + Z_4$	$X_2 + X_4$	$N_1 + N_2$
Band 2	\mathbf{d}_2	\mathbf{d}_4	OK	Γ_5	$P_3 + P_4$	Z_5	$X_1 + X_3$	$N_1 + N_2$
Band 3	\mathbf{d}_3	\mathbf{d}_3	OK	$\Gamma_3 + \Gamma_4$	P_5	$Z_1 + Z_2$	$X_2 + X_4$	$N_1 + N_2$
Band 4	\mathbf{d}_4	\mathbf{d}_2	OK	Γ_5	$P_1 + P_2$	Z_5	$X_1 + X_3$	$N_1 + N_2$

As	$\text{As}(z\bar{z}0)$	$\text{As}(\bar{z}\bar{z}0)$	KI	Γ	P	Z	X	N
Band 1	\mathbf{d}_1	\mathbf{d}_1	OK	$\Gamma_1 + \Gamma_4$	$P_1 + P_4$	$Z_1 + Z_4$	$2X_1$	$N_1 + N_2$
Band 2	\mathbf{d}_2	\mathbf{d}_2	OK	$\Gamma_2 + \Gamma_3$	$P_2 + P_3$	$Z_2 + Z_3$	$2X_3$	$N_1 + N_2$
Band 3	\mathbf{d}_3	\mathbf{d}_4	–	Γ_5	P_5	Z_5	$X_2 + X_4$	$N_1 + N_2$

Ba	$\text{Ba}(000)$	KI	Γ	P	Z	X	N
Band 1	\mathbf{d}_1	OK	Γ_1	P_1	Z_1	X_1	N_1
Band 2	\mathbf{d}_2	OK	Γ_2	P_2	Z_2	X_3	N_2
Band 3	\mathbf{d}_3	OK	Γ_3	P_3	Z_3	X_3	N_1
Band 4	\mathbf{d}_4	OK	Γ_4	P_4	Z_4	X_1	N_2

Notes to Table 3

- (i) $z = 0.36 \dots [1]$; the exact value of z is meaningless in this table.
- (ii) The antiferromagnetic structure of undistorted BaMn_2As_2 has the space group $I\bar{4}2m$ and the magnetic group $M = I\bar{4}2m + \{KI|000\}I\bar{4}2m$ with K denoting the operator of time-inversion.
- (iii) Each row defines a band with Bloch functions that can be unitarily transformed into Wannier functions being
 - as well localized as possible;
 - centered at the stated atoms;
 - and symmetry-adapted to the space group $I\bar{4}2m$ of the antiferromagnetic structure in undistorted BaMn_2As_2 .
- (iv) The notations of the representations are defined in Table 1.
- (v) The bands are determined following Theorem 5 of Ref. [5].
- (vi) The Wannier functions at the Mn, As or Ba atom listed in the upper row belong to the representation \mathbf{d}_i included below the atom.
- (vii) The \mathbf{d}_i denote the one-dimensional representations of the “point groups of the positions” of the Mn, As and Ba atom (Definition 12 of Ref. [5]), S_4 , C_{2v} , and D_{2d} , respectively, as defined by the tables

Mn atoms					As atoms					Ba atom				
$E \ S_{4z}^+ \ C_{2z} \ S_{4z}^-$					$E \ C_{2z} \ \sigma_{da} \ \sigma_{db}$					$S_{4z}^- \ C_{2y} \ \sigma_{da}$				
$E \ S_{4z}^+ \ C_{2z} \ S_{4z}^-$					$E \ C_{2z} \ \sigma_{da} \ \sigma_{db}$					$E \ C_{2z} \ S_{4z}^+ \ C_{2x} \ \sigma_{db}$				
\mathbf{d}_1	1	1	1	1	\mathbf{d}_1	1	1	1	1	\mathbf{d}_1	1	1	1	1
\mathbf{d}_2	1	i	-1	-i	\mathbf{d}_2	1	1	-1	-1	\mathbf{d}_2	1	1	1	-1
\mathbf{d}_3	1	-1	1	-1	\mathbf{d}_3	1	-1	1	-1	\mathbf{d}_3	1	1	-1	1
\mathbf{d}_4	1	-i	-1	i	\mathbf{d}_4	1	-1	-1	1	\mathbf{d}_4	1	1	-1	-1

- (viii) The entry “OK” indicates whether the Wannier functions may even be chosen symmetry-adapted to the magnetic group $M = I\bar{4}2m + \{KI|000\}I\bar{4}2m$ of undistorted BaMn_2As_2 , see Theorem 7 of Ref. [5].
- (ix) Hence, all the listed bands except for band 3 of As form magnetic bands as defined by Definition 16 of Ref. [5].
- (x) Each band consists of one or two branches (Definition 2 of Ref. [5]) depending on the number of the related atoms in the unit cell.

TABLE 4. Character tables of the irreducible representations of the tetragonal space group $P\bar{4}2_1c = \Gamma_q D_{2d}^4$ (114) of the experimentally observed [1] antiferromagnetic structure in distorted BaMn_2As_2 .

$\Gamma(000)$											
K		$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{E 000\}$	$\{C_{2z} 000\}$	$\{S_{4z}^+ 000\}$	$\{C_{2x} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{S_{4z}^- 000\}$	$\{C_{2y} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{\sigma_{da} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{\sigma_{db} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	
Γ_1	(a)	(a)	1	1	1	1	1	1	1	1	
Γ_2	(a)	(a)	1	1	1	-1	-1	-1	-1	-1	
Γ_3	(a)	(a)	1	1	-1	1	1	1	1	1	
Γ_4	(a)	(a)	1	1	-1	-1	-1	-1	-1	-1	
Γ_5	(a)	(a)	2	-2	0	0	0	0	0	0	

$M(\frac{1}{2}\frac{1}{2}0)$											
K		$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{E 000\}$	$\{C_{2z} 010\}$	$\{C_{2z} 000\}$	$\{E 010\}$	$\{\sigma_{db} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{\sigma_{da} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{S_{4z}^+ 000\}$	$\{S_{4z}^- 000\}$	
M_1	(c)	(a)	1	1	-1	-1	1	-1	i	-i	i
M_2	(c)	(a)	1	1	-1	-1	1	-1	-i	i	-i
M_3	(c)	(a)	1	1	-1	-1	-1	1	-i	i	i
M_4	(c)	(a)	1	1	-1	-1	-1	1	i	-i	-i
M_5	(a)	(a)	2	-2	2	-2	0	0	0	0	0

$Z(00\frac{1}{2})$											
K		$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{E 000\}$	$\{C_{2z} 001\}$	$\{C_{2z} 000\}$	$\{E 001\}$	$\{C_{2x} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{2y} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{S_{4z}^+ 000\}$	$\{S_{4z}^- 000\}$	
Z_1	(c)	(a)	1	1	-1	-1	1	-1	i	-i	i
Z_2	(c)	(a)	1	1	-1	-1	1	-1	-i	i	-i
Z_3	(c)	(a)	1	1	-1	-1	-1	1	-i	i	i
Z_4	(c)	(a)	1	1	-1	-1	-1	1	i	-i	-i
Z_5	(a)	(a)	2	-2	2	-2	0	0	0	0	0

$A(\frac{1}{2}\frac{1}{2}\frac{1}{2})$											
K		$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{E 000\}$	$\{C_{2z} 000\}$	$\{E 001\}$	$\{C_{2z} 001\}$	$\{S_{4z}^+ 000\}$	$\{S_{4z}^- 001\}$	$\{\sigma_{da} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{2x} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	
A_1	(c)	(a)	1	1	-1	-1	-1	1	i	-i	i
A_2	(c)	(a)	1	1	-1	-1	-1	1	-i	i	-i
A_3	(c)	(a)	1	1	-1	-1	1	-1	-i	-i	i
A_4	(c)	(a)	1	1	-1	-1	1	-1	i	i	-i
A_5	(b)	(a)	2	-2	-2	2	0	0	0	0	0

$R(0\frac{1}{2}\frac{1}{2})$						$X(0\frac{1}{2}0)$					
$\{E 000\}$		$\{E 001\}$	$\{C_{2y} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{2z} 000\}$	$\{C_{2x} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{E 000\}$		$\{E 010\}$	$\{C_{2y} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{2z} 000\}$	$\{C_{2x} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
R_1	2	-2	0	0	0	X_1	2	-2	0	0	0

Notes to Table 4

- (i) The notations of the points of symmetry follow Fig. 3.9 of Ref. [9].
- (ii) The character tables are determined from Table 5.7 of Ref. [9].
- (iii) K denotes the operator of time inversion. The entries (a), (b) and (c) indicate whether the related co-representations of the magnetic groups $P\bar{4}2_1c + \{K|000\}P\bar{4}2_1c$ and $P\bar{4}2_1c + \{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}P\bar{4}2_1c$ follow case (a), (b) or (c) as defined in equations (7.3.45), (7.3.46) and (7.3.47), respectively, of Ref. [9] (and determined by equation (7.3.51) of Ref. [9]). This information is interesting only in symmetry points invariant under the complete space group.
- (iv) The entries (a) and (c) for K and $\{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ show that all the one-dimensional representations at M , Z , or A are possible representations of a *stable* antiferromagnetic state, see Appendix A of Ref. [16] or Section III C of Ref. [14].

TABLE 5. Compatibility relations between the Brillouin zone for the space group $I4/mmm$ (139) of tetragonal paramagnetic BaMn_2As_2 and the Brillouin zone for the space group $P\bar{4}2_1c$ (114) of the antiferromagnetic structure in distorted BaMn_2As_2 .

$\Gamma(000)$											$X(00\frac{1}{2})$							
Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-		X_1^+	X_2^+	X_3^+	X_4^+	X_1^-	X_2^-	X_3^-	X_4^-
Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_3	Γ_4	Γ_1	Γ_2	Γ_5		M_5	$M_1 + M_2$	M_5	$M_3 + M_4$	M_5	$M_3 + M_4$	M_5	$M_1 + M_2$

$Z(\frac{1}{2}\frac{1}{2}\frac{1}{2})$											$P(\frac{1}{4}\frac{1}{4}\frac{1}{4})$				
Z_1^+	Z_2^+	Z_3^+	Z_4^+	Z_5^+	Z_1^-	Z_2^-	Z_3^-	Z_4^-	Z_5^-		P_1	P_2	P_3	P_4	P_5
Γ_2	Γ_1	Γ_4	Γ_3	Γ_5	Γ_4	Γ_3	Γ_2	Γ_1	Γ_5		$A_3 + A_4$	$A_3 + A_4$	$A_1 + A_2$	$A_1 + A_2$	$2A_5$

$\Lambda_M(\frac{1}{4}\frac{1}{4}\frac{1}{4})$											line Λ	
Λ_1	Λ_2	Λ_3	Λ_4								Λ_5	
Z_5	Z_5	Z_5	Z_5	Z_1	Z_2	Z_3	Z_4					

Notes to Table 5

- (i) The Brillouin zone for $P\bar{4}2_1c$ lies within the Brillouin zone for $I4/mmm$.
- (ii) The upper rows list the representations of the little groups of the points of symmetry in the Brillouin zone for $I4/mmm$ and the lower rows list representations of the little groups of the related points of symmetry in the Brillouin zone for $P\bar{4}2_1c$.
The representations in the same column are compatible in the following sense: Bloch functions that are basis functions of a representation \mathbf{D}_i in the upper row can be unitarily transformed into the basis functions of the representation given below \mathbf{D}_i .
- (iii) The notations of the representations are defined in Table 2 of Ref. [13] and Table 4, respectively.
- (iv) $\Lambda_M(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ denotes the midpoint between Γ and Z in the Brillouin zone for $I4/mmm$.
- (v) The representations on the line Λ in the Brillouin zone for $I4/mmm$ are simple: the branch connecting Γ_5 and Z_5 in Fig.2 is labeled by the two-dimensional representation Λ_5 , all the other branches are labeled by one of the one-dimensional representations Λ_1 , Λ_2 , Λ_3 , or Λ_4 .
- (vi) The compatibility relations are determined in the way described in great detail in Ref. [17].

TABLE 6. Representations at the points of symmetry in the space group $P\bar{4}2_1c$ (114) of all the energy bands of *distorted* antiferromagnetic BaMn_2As_2 with symmetry-adapted and optimally localized Wannier functions centered at the Mn, As, or Ba atoms, respectively.

Mn	$\text{Mn}(\frac{1}{2}0\frac{1}{4})$	$\text{Mn}(0\frac{1}{2}\frac{1}{4})$	$\text{Mn}(1\frac{1}{2}\frac{3}{4})$	$\text{Mn}(\frac{1}{2}1\frac{3}{4})$	$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	Γ	M
Band 1	\mathbf{d}_1	\mathbf{d}_1	\mathbf{d}_1	\mathbf{d}_1	OK	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$	$M_1 + M_2 + M_3 + M_4$
Band 2	\mathbf{d}_2	\mathbf{d}_2	\mathbf{d}_2	\mathbf{d}_2	*	$2\Gamma_5$	$2M_5$

(continued)

Mn	Z	A	R	X
Band 1	$2Z_5$	$2A_5$	$2R_1$	$2X_1$
Band 2	$Z_1 + Z_2 + Z_3 + Z_4$	$A_1 + A_2 + A_3 + A_4$	$2R_1$	$2X_1$

As	$\text{As}(00z)$	$\text{As}(00\bar{z})$	$\text{As}(\frac{1}{2}\frac{1}{2}, \frac{1}{2} + z)$	$\text{As}(\frac{1}{2}\frac{1}{2}, \frac{1}{2} - z)$	$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	Γ	M
Band 1	\mathbf{d}_1	\mathbf{d}_1	\mathbf{d}_1	\mathbf{d}_1	OK	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$	$2M_5$
Band 2	\mathbf{d}_2	\mathbf{d}_2	\mathbf{d}_2	\mathbf{d}_2	*	$2\Gamma_5$	$M_1 + M_2 + M_3 + M_4$

(continued)

As	Z	A	R	X
Band 1	$2Z_5$	$A_1 + A_2 + A_3 + A_4$	$2R_1$	$2X_1$
Band 2	$Z_1 + Z_2 + Z_3 + Z_4$	$2A_5$	$2R_1$	$2X_1$

Ba	$\text{Ba}(000)$	$\text{Ba}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$\{KI \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	Γ	M	Z	A	R	X
Band 1	\mathbf{d}_1	\mathbf{d}_1	OK	$\Gamma_1 + \Gamma_2$	M_5	Z_5	$A_3 + A_4$	R_1	X_1
Band 2	\mathbf{d}_2	\mathbf{d}_4	OK	Γ_5	$M_1 + M_4$	$Z_1 + Z_4$	A_5	R_1	X_1
Band 3	\mathbf{d}_3	\mathbf{d}_3	OK	$\Gamma_3 + \Gamma_4$	M_5	Z_5	$A_1 + A_2$	R_1	X_1
Band 4	\mathbf{d}_4	\mathbf{d}_2	OK	Γ_5	$M_2 + M_3$	$Z_2 + Z_3$	A_5	R_1	X_1

Notes to Table 6

- (i) $z = 0.36 \dots$ [1]; the exact value of z is meaningless in this table.
- (ii) The space group $P\bar{4}2_1c$ leaves invariant the experimentally observed [1] antiferromagnetic structure and defines the distortion of BaMn_2As_2 that possesses the magnetic super band consisting of band 1 of Mn, band 2 of As, and band 3 of Ba.
- (iii) The appertaining magnetic group reads as $M = P\bar{4}2_1c + \{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}P\bar{4}2_1c$, where K still denotes the operator of time-inversion.
- (iv) The notations of the representations are defined in Table 4.
- (v) The bands are determined following Theorem 5 of Ref. [5].
- (vi) Each row defines a band with Bloch functions that can be unitarily transformed into Wannier functions being
 - as well localized as possible;
 - centered at the stated atoms; and
 - symmetry-adapted to $P\bar{4}2_1c$.

Notes to Table 6 (continued)

- (vii) The Wannier functions at the Mn, As or Ba atom listed in the upper row belong to the representation \mathbf{d}_i included below the atom.
- (viii) The \mathbf{d}_i denote the representations of the “point groups of the positions” of the Mn, As and Ba atoms (Definition 12 of Ref. [5]), C_2 , C_2 , and S_4 , respectively, as defined by the tables

Mn atoms			As atoms			Ba atoms			
$\{E 000\}$	$\{C_{2z} 000\}$		$\{E 000\}$	$\{C_{2z} 000\}$		$\{E 000\}$	$\{S_{4z}^+ 000\}$	$\{C_{2z} 000\}$	$\{S_{4z}^- 000\}$
\mathbf{d}_1	1	1	\mathbf{d}_1	1	1	\mathbf{d}_1	1	1	1
\mathbf{d}_2	1	-1	\mathbf{d}_2	1	-1	\mathbf{d}_2	1	i	-1
						\mathbf{d}_3	1	-1	1
						\mathbf{d}_4	1	-i	-1

- (ix) The entry “OK” indicates whether the Wannier functions may even be chosen symmetry-adapted to the magnetic group $M = P\bar{4}2_1c + \{KI|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}P\bar{4}2_1c$, see Theorem 7 of Ref. [5].
- (x) The asterisk “*” indicates that the Wannier functions may be chosen symmetry-adapted to the magnetic group M , but they do not allow that the magnetic moments are situated at the appertaining atoms. This complication (which has not yet been considered in Ref. [5]) may (but does not necessarily) occur only if the representations of the space group at point Γ are not one-dimensional as it is the case in band 2 of both Mn and As, and in bands 2 and 4 of Ba. Consider, for example, band 2 of Mn and the two $\text{Mn}(\frac{1}{2}0\frac{1}{4})$ and $\text{Mn}(\frac{1}{2}1\frac{3}{4})$ atoms. The magnetic moments at the two positions A and B of these atoms are anti-parallel. Thus, the two Wannier functions $w_A(\vec{r})$ and $w_B(\vec{r})$ at these positions are complex conjugate, $w_A(\vec{r}) = w_B^*(\vec{r})$, and, hence, belong to co-representations \mathbf{d}_A and \mathbf{d}_B of the groups of these positions being also complex conjugate,

$$\mathbf{d}_A = \mathbf{d}_B^*. \quad (\text{A.1})$$

The matrix \mathbf{N} defined by Theorem 7 of Ref. [5] takes the form $\mathbf{N} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ in band 2 of Mn, yielding the two co-representations \mathbf{d}_A and \mathbf{d}_B defined by the table

	E	C_{2z}	$K\sigma_x$	$K\sigma_y$
\mathbf{d}_A	1	-1	1	-1
\mathbf{d}_B	1	-1	-1	1

Because \mathbf{d}_A and \mathbf{d}_B do not comply with Equation (A.1), the Wannier functions defined by band 2 of Mn do not form a magnetic band in antiferromagnetic BaMn_2As_2 since it is experimentally proven that the ordered magnetic moments lie at the Mn atoms. The Wannier functions defined by band 2 of As, on the other hand, form a magnetic band in BaMn_2As_2 because the As atoms do not bear ordered magnetic moments.

- (xi) Each band consists of two or four branches (Definition 2 of Ref. [5]) depending on the number of the related atoms in the unit cell.

TABLE 7. Character tables of the single-valued irreducible representations of the tetragonal space group $P\overline{4} = \Gamma_q S_4^1$ (81).
$$\Gamma(000), M(\frac{1}{2}\frac{1}{2}0), Z(00\frac{1}{2}), A(\frac{1}{2}\frac{1}{2}\frac{1}{2})$$

		K	KC_{2a}	E	S_{4z}^+	C_{2z}	S_{4z}^-
R_1	(a)	(a)		1	1	1	1
R_2	(c)	(a)		1	i	-1	-i
R_3	(a)	(a)		1	-1	1	-1
R_4	(c)	(a)		1	-i	-1	i

Notes to Table 7

- (i) The notations of the points of symmetry follow Fig. 3.9 of Ref. [9].
- (ii) Only the points of symmetry invariant under the complete space group are listed.
- (iii) The character tables are determined from Table 5.7 in Ref. [9].
- (iv) K still denotes the operator of time inversion. The entries (a) and (c) indicate whether the related corepresentations of the magnetic groups $P\overline{4} + \{K|000\}P\overline{4}$ and $P\overline{4} + \{KC_{2a}|000\}P\overline{4}$ follow case (a) or case (c) as defined in equations (7.3.45) and (7.3.47), respectively, of Ref. [9] (and determined by equation (7.3.51) of Ref. [9]).
- (v) The entries (a) and (c) for K and KC_{2a} show that the representations R_2 and R_4 at any of the points Γ , M , Z , or A are possible representations of a *stable* antiferromagnetic state, see Appendix A of Ref. [16] or Section III C of Ref. [14]. This is important since M_{81} (6) is the *exact* group of the magnetic structure in BaMn_2As_2 .

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